Supplementary Materials: Influence of Substituents in Terephthalate Linker on the Structure of MOFs Obtained from Presynthesized Heterometallic Complex

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Table S1. List of selected angles and bond distances for starting complex and compounds **1**–**4**.

Compound	Bond distances, Å	Angles, deg.
$[Li_2Zn_2(piv)_6(py)_2]$	Zn(1) – O(3) 1.9297(18) Zn(1) – O(5) 1.951(2) Zn(1) – O(1) 1.9519(19) Zn(1) – N(1) 2.067(2) Li(1) – O(4) 1.889(5) Li(1) – O(1) 1.902(5) Li(1) – O(2) 1.936(5) Li(1) – O(2) 1.985(5)	O(3) – Zn(1) – N(1) 95.82(8) O(1) – Zn(1) – N(1) 96.91(9) O(5) – Zn(1) – N(1) 103.61(9) O(1) – Zn(1) – O(5) 102.77(9) O(1) – Zn(1) – O(2) 120.42(8) O(3) – Zn(1) – O(5) 129.78(10) O(2) – Li(1) –O(2) 94.4(2) O(2) – Li(1) – O(6) 102.6(2) O(4) – Li(1) – O(6) 109.4(2) O(2) – Li(1) –O(4) 112.0(3) O(2) – Li(1) – O(6) 116.0(3) O(2) – Li(1) – O(4) 120.1(3) Li(1) –O(2) – Li(1) 85.6(2)
1	Zn(1) – O(21) 1.944(2) Zn(1) – O(31) 1.952(2) Zn(1) – O(33) 1.961(2) Zn(1) – O(11) 1.974(2) Li(1) – O(32) 1.860(6) Li(1) – O(34) 1.883(6) Li(1) – O(22) 1.944(6) Li(1) – O(22) 1.953(6)	O(11) – Zn(1) – O(33) 98.60(11) O(11) – Zn(1) – O(31) 104.89(11) O(31) – Zn(1) – O(33) 107.47(12) O(11) – Zn(1) – O(21) 108.26(11) O(21) – Zn(1) – O(33) 108.49(11) O(21) – Zn(1) – O(31) 125.76(11) O(22) – Li(1) – O(22) 94.4(2) O(32) – Li(1) – O(34) 108.5(3) O(22) – Li(1) – O(32) 111.6(3) O(22) – Li(1) – O(32) 112.2(3) O(22) – Li(1) – O(34) 113.8(3) O(22) – Li(1) – O(34) 115.9(3) Li(1) – O(22) – Li(1) 85.6(2)
2$_{DMA}$	Zn(1) – O(31) 1.933(4) Zn(1) – O(21) 1.933(5) Zn(1) – O(42) 1.943(4) Zn(1) – O(12) 1.984(4) Li(1) – O(11) 1.879(13) Li(1) – O(22) 1.885(12) Li(1) – O(41) 1.921(12) Li(1) – O(41) 1.956(12)	O(31) – Zn(1) – O(42) 96.41(18) O(12) – Zn(1) – O(31) 96.59(19) O(12) – Zn(1) – O(21) 112.4(2) O(12) – Zn(1) – O(42) 114.7(2) O(21) – Zn(1) – O(42) 116.4(2) O(21) – Zn(1) – O(31) 117.96(19) O(41) – Li(1) – O(41) 92.0(5) O(11) – Li(1) – O(22) 106.5(6) O(11) – Li(1) – O(41) 107.1(6) O(11) – Li(1) – O(41) 113.2(6) O(22) – Li(1) – O(41) 116.2(6) O(22) – Li(1) – O(41) 120.9(6) Li(1) – O(41) – Li(1) 88.0(5)
3	Zn(1) – O(101) 1.922(2) Zn(1) – O(103) 1.929(2) Zn(1) – O(201) 1.960(2)	O(101) – Zn(1) – O(202) 92.84(10) O(103) – Zn(1) – O(202) 98.84(10) O(103) – Zn(1) – O(201) 100.92(10)

	Zn(1) – O(202) 2.001(2)	O(101) – Zn(1) – O(201) 113.94(11)
	Li(1) – O(104) 1.890(5)	O(201) – Zn(1) – O(202) 118.95(10)
	Li(1) – O(102) 1.907(5)	O(101) – Zn(1) – O(103) 131.50(11)
		O(102) – Li(1) – O(102) 104.2(4)
		O(104) – Li(1) – O(104) 105.7(4)
		O(102) – Li(1) – O(104) 108.03(12)
		O(102) – Li(1) – O(104) 115.58(11)
		O(11) – Zn(1) – O(1D) 77.44(19)
		O(22) – Zn(1) – O(1D) 78.51(19)
		O(1D) – Zn(1) – N(1P) 90.78(17)
		O(11) – Zn(1) – O(32) 98.46(12)
		O(32) – Zn(1) – N(1P) 98.77(11)
		O(11) – Zn(1) – N(1P) 101.36(11)
	Zn(1) – O(22) 1.943(3)	O(22) – Zn(1) – O(32) 101.46(13)
	Zn(1) – O(11) 1.968(2)	O(22) – Zn(1) – N(1P) 101.56(12)
	Zn(1) – O(32) 2.008(2)	O(11) – Zn(1) – O(22) 146.76(13)
	Zn(1) – N(1P) 2.030(3)	O(32) – Zn(1) – O(1D) 170.22(17)
	Zn(1) – O(1D) 2.303(5)	O(12) – Li(1) – O(12) 94.0(2)
	Li(1) – O(21) 1.865(6)	O(21) – Li(1) – O(31) 108.6(3)
	Li(1) – O(31) 1.901(6)	O(12) – Li(1) – O(21) 112.4(3)
	Li(1) – O(12) 1.927(6)	O(12) – Li(1) – O(31) 112.4(3)
4	Li(1) – O(12) 1.955(6)	O(12) – Li(1) – O(31) 114.0(3)
	Zn(2) – O(34) 1.915(3)	O(21) – Li(1) – O(12) 115.0(3)
	Zn(2) – O(24) 1.923(3)	Li(1) – O(12) – Li(1) 86.0(2)
	Zn(2) – O(13) 1.925(2)	O(34) – Zn(2) – O(2D) 97.20(13)
	Zn(2) – O(2D) 1.971(3)	O(24) – Zn(2) – O(2D) 102.15(12)
	Li(2) – O(14) 1.892(3)	O(13) – Zn(2) – O(2D) 107.25(12)
	Li(2) – O(23) 1.904(3)	O(13) – Zn(2) – O(24) 113.69(12)
	Li(2) – O(33) 1.910(3)	O(24) – Zn(2) – O(34) 113.75(14)
	Li(2) – O(3D) 1.967(3)	O(13) – Zn(2) – O(34) 119.46(13)
		O(14) – Li(2) – O(3D) 102.47(14)
		O(33) – Li(2) – O(3D) 105.39(16)
		O(23) – Li(2) – O(33) 109.25(15)
		O(23) – Li(2) – O(3D) 112.07(14)
		O(14) – Li(2) – O(23) 113.27(14)
		O(14) – Li(2) – O(33) 113.98(17)

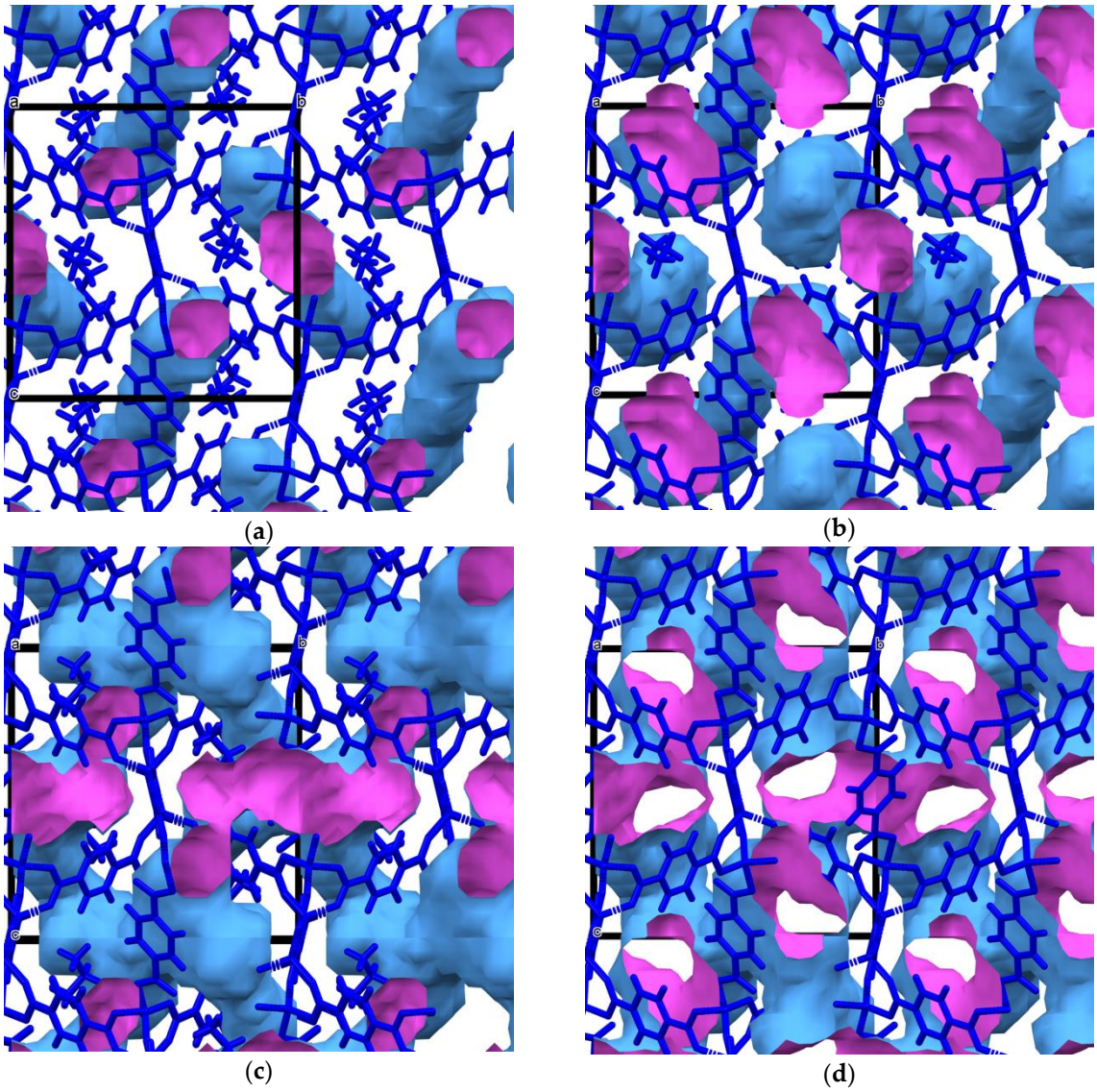
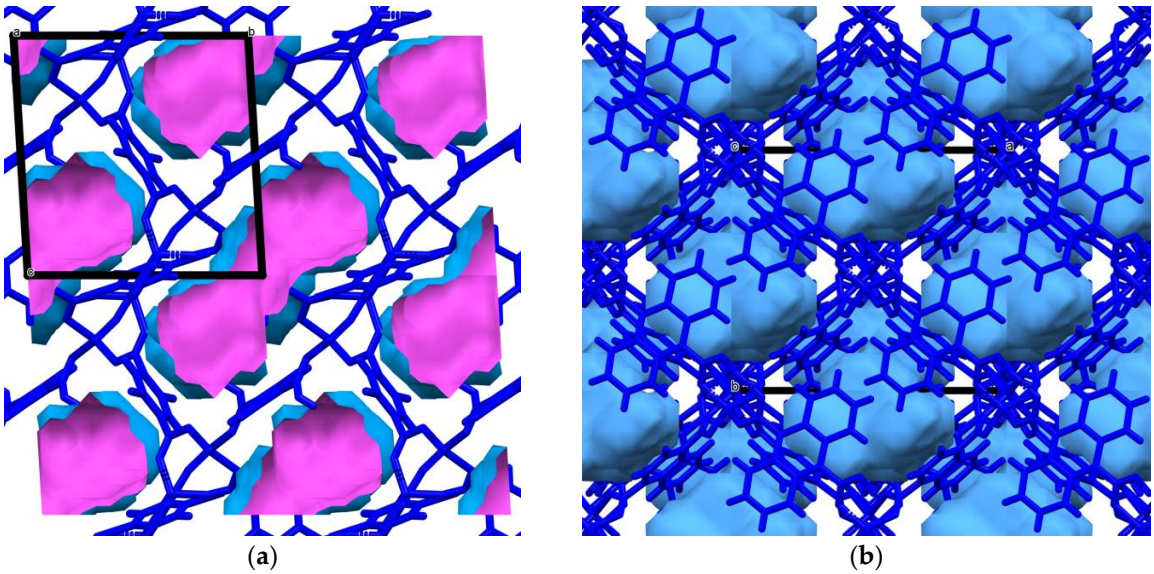
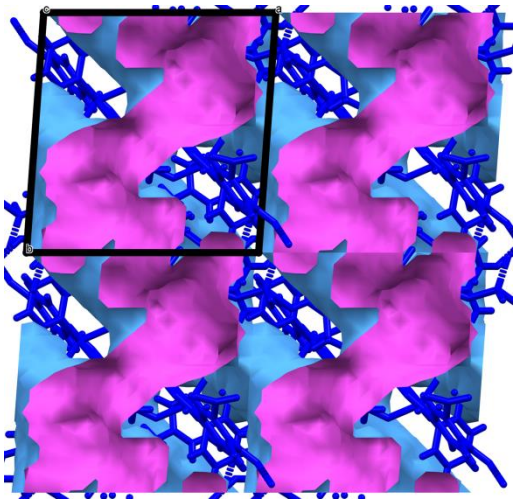


Figure S1. (**a**) Pore representation in **1** with both disordered counterions; (**b**) Pore representation in **1** with the first type of partly occupied counterions fixed; (**c**) Pore representation in **1** the second type of partly occupied counterions fixed; (**d**) Pore representation in **1** without all counterions. Pore inner surface is shown in pink, outer surface – in blue. Framework and counterions are shown in dark blue.





(**c**)

Figure S2. (**a**) Pore representation in **2**; (**b**) Pore representation in **3**; (**c**) Pore representation in **4**. Pore inner surface is shown in pink, outer surface – in blue. Framework is shown in dark blue.

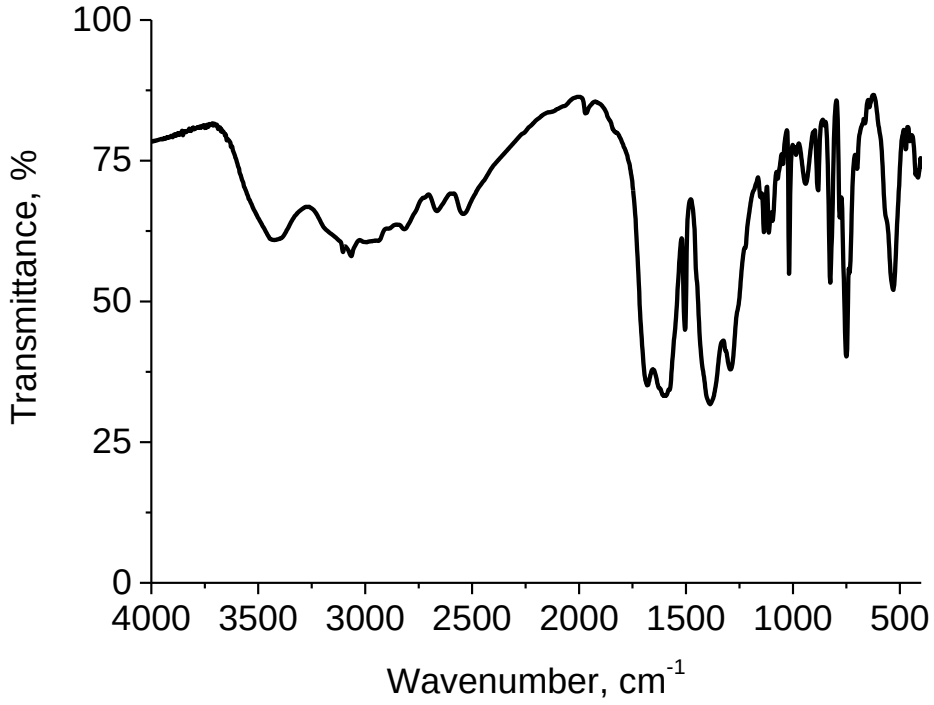


Figure S3. IR spectrum of compound **1**.

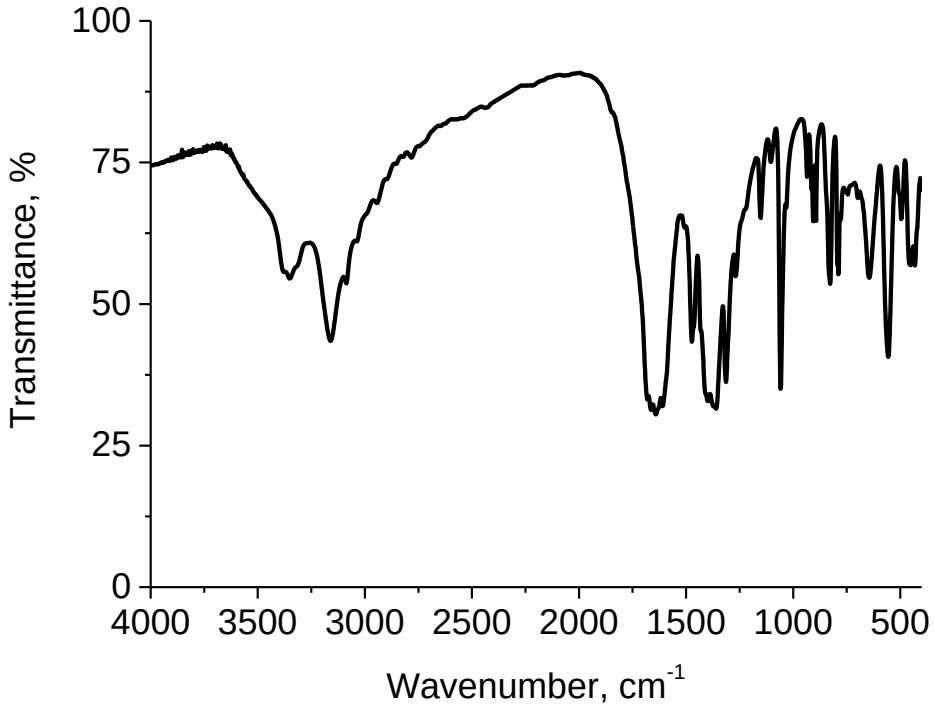


Figure S4. IR spectrum of compound **2**.

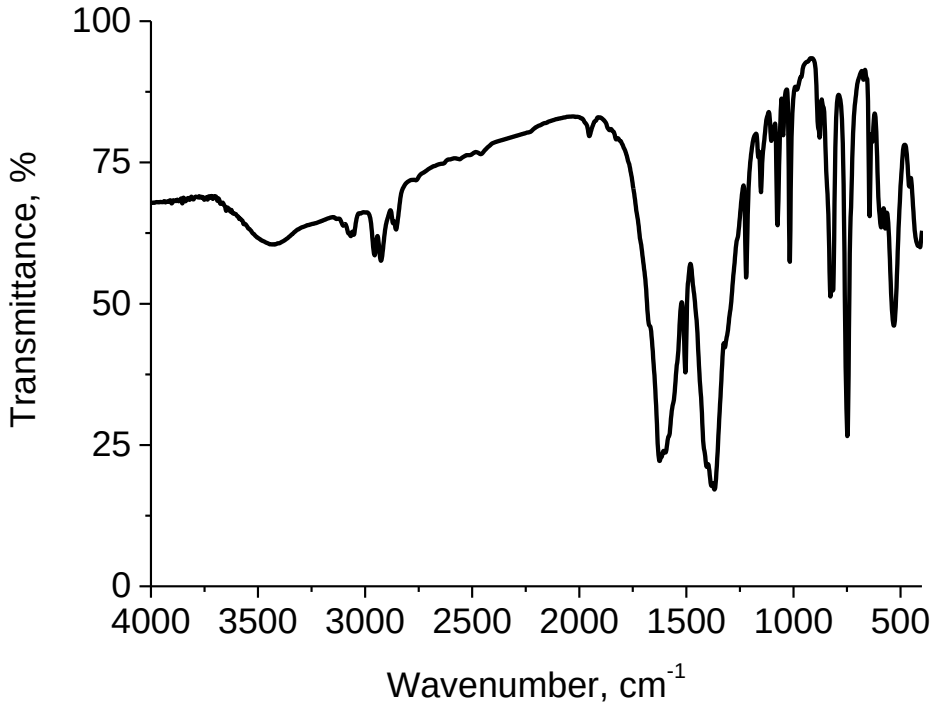


Figure S5. IR spectrum of compound **3**.